Butyl 2-bromobutanoate

Other names: butyl 2-bromobutyrate
Inchi: InChI=1S/C8H15BrO2/c1-3-5-6-11-8(10)7(9)4-2/h7H,3-6H2,1-2H3
InchiKey: DKZLMRKANVHJGG-UHFFFAOYSA-N
Formula: C8H15BrO2
SMILES: CCCCOC(=O)C(Br)CC
Mol. weight [g/mol]: 223.11
CAS: 42115-48-0

Physical Properties

Property code	Value	Unit	Source
gf	-205.56	kJ/mol	Joback Method
hf	-432.20	kJ/mol	Joback Method
hfus	21.02	kJ/mol	Joback Method
hvap	48.61	kJ/mol	Joback Method
log10ws	-2.58		Crippen Method
logp	2.503		Crippen Method
mcvol	148.520	ml/mol	McGowan Method
pc	2881.21	kPa	Joback Method
rinpol	1182.00		NIST Webbook
rinpol	1182.00		NIST Webbook
tb	524.45	K	Joback Method
tc	718.18	K	Joback Method
tf	296.88	K	Joback Method
vc	0.564	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	320.63	J/mol×K	524.45	Joback Method
cpg	332.86	J/mol×K	556.74	Joback Method
cpg	344.53	J/mol×K	589.03	Joback Method
cpg	355.66	J/mol×K	621.31	Joback Method
cpg	366.25	J/mol×K	653.60	Joback Method
cpg	376.32	J/mol×K	685.89	Joback Method

cpg	385.87	J/mol×K	718.18	Joback Method
dvisc	0.0033286	Pa×s	296.88	Joback Method
dvisc	0.0017041	Pa×s	334.81	Joback Method
dvisc	0.0009998	Pa×s	372.74	Joback Method
dvisc	0.0006473	Pa×s	410.67	Joback Method
dvisc	0.0004510	Pa×s	448.59	Joback Method
dvisc	0.0003325	Pa×s	486.52	Joback Method
dvisc	0.0002562	Pa×s	524.45	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C42115480&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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